FILE 'REGISTRY' ENTERED AT 14:06:05 ON 12 JUN 2003

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 JUN 2003 HIGHEST RN 529474-19-9
DICTIONARY FILE UPDATES: 11 JUN 2003 HIGHEST RN 529474-19-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

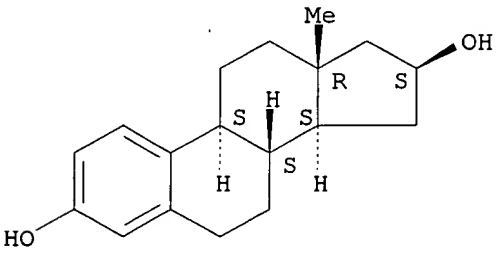
Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> s 1225-58-7/rn
L10 1 1225-58-7/RN

=> d l10

L10 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS
RN **1225-58-7** REGISTRY
CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estra-1,3,5(10)-triene-3,16.beta.-diol (6CI, 7CI, 8CI)
OTHER NAMES:
CN 16.beta.-Estradiol
CN 3,16.beta.-Dihydroxyestra-1,3,5,(10)-triene
FS STEREOSEARCH
MF C18 H24 O2
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CSCHEM, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

17 REFERENCES IN FILE CA (1957 TO DATE)
17 REFERENCES IN FILE CAPLUS (1957 TO DATE)
5 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.08	71.42

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-5.85

FILE 'CAPLUS' ENTERED AT 14:06:47 ON 12 JUN 2003
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FILE COVERS 1907 - 12 Jun 2003 VOL 138 ISS 24
FILE LAST UPDATED: 11 Jun 2003 (20030611/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l10
L11 17 L10

=> d l11 1-4 ibib hitstr abs

L11 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:552017 CAPLUS
DOCUMENT NUMBER: 133:150782
TITLE: synthesis of 16-Hydroxyestratrienes as selectively effective estrogens
INVENTOR(S): Kuenzer, Hermann; Knauthe, Rudolf; Lessl, Monika; Fritzemeier, Karl-heinrich; Hegele-Hartung, Christa; Boemer, Ulf; Mueller, Gerd; Kosemund, Dirk
PATENT ASSIGNEE(S): Schering A.-G., Germany
SOURCE: Ger. Offen., 34 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19906159	A1	20000810	DE 1999-19906159	19990209
CA 2359660	AA	20000817	CA 2000-2359660	20000209
WO 2000047603	A2	20000817	WO 2000-EP1073	20000209
WO 2000047603	A3	20010802		
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
AU 2000029095	A5	20000829	AU 2000-29095	20000209
EP 1144431	A2	20011017	EP 2000-907539	20000209
EP 1144431	A3	20020612		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
BR 2000008076	A	20020205	BR 2000-8076	20000209
JP 2002536455	T2	20021029	JP 2000-598520	20000209
EE 200100412	A	20021216	EE 2001-412	20000209
NO 2001003860	A	20011008	NO 2001-3860	20010808
BG 105804	A	20020329	BG 2001-105804	20010809

PRIORITY APPLN. INFO.: DE 1999-19906159 A 19990209
WO 2000-EP1073 W 20000209

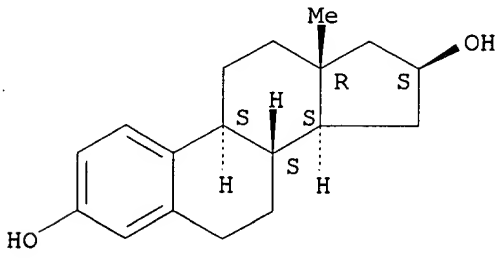
OTHER SOURCE(S): MARPAT 133:150782

IT **1225-58-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of 16-Hydroxyestratrienes as selectively effective estrogens)

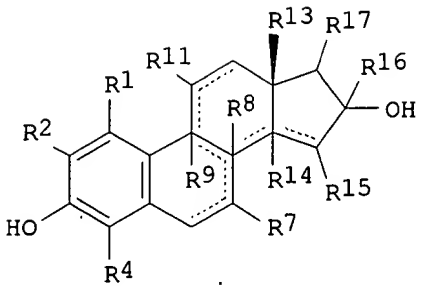
RN 1225-58-7 CAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



GI

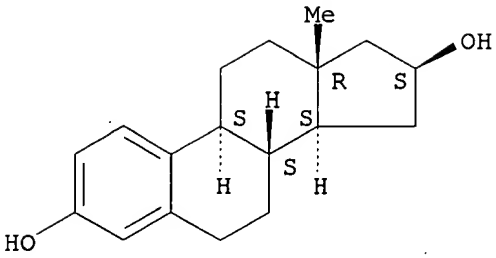


I

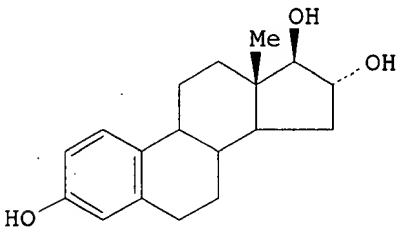
AB Synthesis of 16-Hydroxyestratrienes (I) [R1 = halogen, HO, Me, F3C, MeO, EtO, H; R2 = halogen, HO, (un)substituted alkoxy, H; R4 = halogen, fluoroalkyl, F3C, F5C2, (un)substituted alkoxy, H; R7 = halogen, (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkoxy, (un)substituted heteroaryl, (un)substituted aryl, H; R8 = H, fluoroalkyl, fluoroalkenyl, CN; R9 = H, Me, Et, F3C, F5C2; R11 = NO2O, HO, HS, halogen, chloromethyl, fluoroalkenyl, fluoroalkyl, (un)substituted alkoxy, (un)substituted alkylthio, (un)substituted aryl, (un)substituted heteroaryl, H; R13 = Me, Et, F3C, F5C2; R14 = (un)substituted alkenyl, (un)substituted alkyl, H; R15 = halogen, fluoroalkyl, fluoroalkenyl, =O, =S, SO, SO2, (un)substituted =NH; R14, R15 together = methylene; R16 = fluoroalkyl, fluoroalkenyl, F3C, F5C2,CN, H; R17 = fluoroalkyl, fluoroalkenyl, H, HO] as selectively effective estrogens is disclosed. Thus, 16.alpha.-estradiol shows a 50% uterine stimulation at 30 .upsilon.g in in vivo testing.

L11 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1990:801 CAPLUS
DOCUMENT NUMBER: 112:801
TITLE: Relative mitogenic activities of various estrogens and antiestrogens
AUTHOR(S): Stack, Gary; Korach, Kenneth; Gorski, Jack
CORPORATE SOURCE: Coll. Agric. Life Sci., Univ. Wisconsin, Madison, WI, 53706, USA
SOURCE: Steroids (1989), 54(2), 227-43
CODEN: STEDAM; ISSN: 0039-128X
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **1225-58-7**, 16.beta.-Estradiol
RL: PROC (Process)
(mitogenic action of, on uterus, mol. structure in relation to)
RN 1225-58-7 CAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

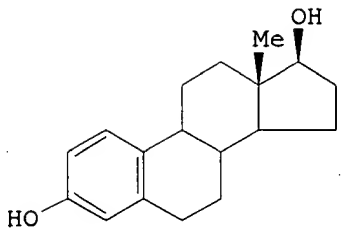
Absolute stereochemistry.



GI



I



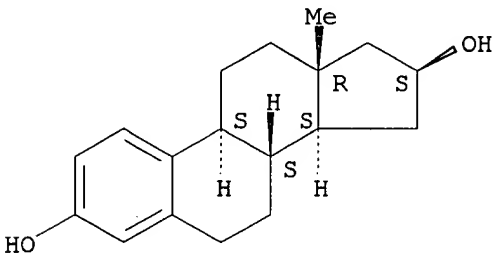
II

AB The abilities of a variety of estrogens and antiestrogens to stimulate DNA synthesis in the prepuberal rat uterus were compared. One microgram of each compd. was administered in vivo via a single i.p. injection. DNA synthesis was assayed in vitro in isolated nuclei 24 h later. The relative mitogenicities of the steroidal estrogens were : 16.alpha.-estradiol < 17.alpha.-estradiol = estriol (I) = 16-epiestriol < 16.beta.-estradiol = 17.beta.-estradiol (II). The potencies of several nonsteroidal estrogens were also tested. Indenestrol A was as potent as II, whereas indanestrol and dimethylstilbestrol had weaker activities. The antiestrogens, nafoxidine and 4-hydroxytamoxifen, were both potent stimulators of DNA synthesis. The abilities of an estrogen to stimulate increases in uterine wet wt., DNA polymerase .alpha. activities, and DNA synthesis in uterine nuclei 24 h after injection were closely correlated. Because the magnitude of the stimulation of DNA synthesis was greatest, its measurement is the most sensitive of these assays, of uterotropic activity.

L11 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1988:622771 CAPLUS
DOCUMENT NUMBER: 109:222771
TITLE: Effect of endogenous and synthetic sex steroids on the clearance of antibody-coated cells
AUTHOR(S): Schreiber, A. D.; Nettl, F. M.; Sanders, M. C.; King, M.; Szabolcs, P.; Friedman, D.; Gomez, F.
CORPORATE SOURCE: Cancer Cent., Univ. Pennsylvania, Philadelphia, PA, 19104, USA
SOURCE: Journal of Immunology (1988), 141(9), 2959-66
CODEN: JOIMA3; ISSN: 0022-1767
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **1225-58-7**
RL: BIOL (Biological study)

(IgG-coated erythrocyte clearance by spleen macrophage stimulation by)
RN 1225-58-7 CAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

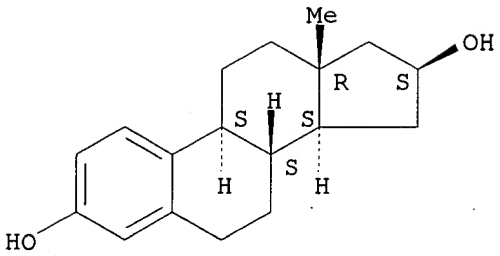
Absolute stereochemistry.



AB An exptl. model developed in the guinea pig, was used to study the effects of female sex hormones on macrophage clearance of IgG- and IgM-coated erythrocytes in the spleen and liver. Progesterone, its naturally occurring analog 17-hydroxyprogesterone, and its synthetic analog 16-methylprogesterone inhibited the clearance of IgG-coated erythrocytes by splenic macrophages. Furthermore, when splenic macrophages were isolated from progesterone-treated animals they expressed decreased Fc.gamma.R activity. Estradiol, estriol, and the estrogen analog 1,3,5(10)-estratriene-3,16.beta.-diol enhanced splenic macrophage clearance of IgG-coated erythrocytes. This action of the estrogens could be partially inhibited by the antiestrogen tamoxifen. However, estradiol did not affect the C3-dependent clearance of IgM-coated erythrocytes by hepatic macrophages. Concurrent administration of estradiol and progesterone demonstrated that the action of estradiol was predominant. Thus, female sex hormones alter splenic macrophage Fc.gamma.R function at concns. obsd. during the human menstrual cycle and pregnancy. This result may also explain alteration of disease activity in some human immunol. disorders during changes in the hormonal states.

L11 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1987:96443 CAPLUS
DOCUMENT NUMBER: 106:96443
TITLE: Influence of adrenergic receptors on ovarian progesterone secretion in the pseudopregnant cat and estradiol secretion in the estrous cat
AUTHOR(S): Wheeler, A. G.; Walker, M.; Lean, J.
CORPORATE SOURCE: Dep. Physiol. Pharmacol., Univ. Queensland, St. Lucia, 4067, Australia
SOURCE: Journal of Reproduction and Fertility (1987), 79(1), 195-205
CODEN: JRPFA4; ISSN: 0022-4251
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **1225-58-7**
RL: PROC (Process)
(secretion of, by ovary, adrenergic receptors in relation to)
RN 1225-58-7 CAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB The infusion of isoprenaline [7683-59-2] or propranolol into the abdominal aorta of the pseudopregnant cat caused an increase or decrease, resp., in the ovarian progesterone [57-83-0] secretion rate. Apparently, the sympathetic innervation of the ovary has a physiol. influence on normal progesterone secretion, and this mechanism may explain stress-related increases in progesterone concns. The infusion of isoprenaline or propranolol after the stimulation of follicular growth had no consistent or convincing effect on estradiol [**1225-58-7**] secretion.

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=> d l10 5-17 ibib hitstr abs
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y


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The answer numbers requested are not in the answer set.
ENTER ANSWER NUMBER OR RANGE (1):5-17
     1 ANSWERS ARE AVAILABLE.  SPECIFIED ANSWER NUMBER EXCEEDS ANSWER SET SIZE
The answer numbers requested are not in the answer set.
ENTER ANSWER NUMBER OR RANGE (1):end

=> d his

     (FILE 'HOME' ENTERED AT 13:10:32 ON 12 JUN 2003)

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L1             1 S 28834-40-4/RN
L2             1 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 13:12:23 ON 12 JUN 2003
L3             3 S L2

     FILE 'REGISTRY' ENTERED AT 13:17:42 ON 12 JUN 2003
L4               STR 28834-40-4
L5             0 S L4 FAM SAM

     FILE 'REGISTRY' ENTERED AT 14:03:13 ON 12 JUN 2003
L6             1 S 16 ALPHA ESTRADIOL

     FILE 'CAPLUS' ENTERED AT 14:03:51 ON 12 JUN 2003
L7             3 S L1

     FILE 'REGISTRY' ENTERED AT 14:04:32 ON 12 JUN 2003
L8             1 S 1090-04-6/RN
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FILE 'CAPLUS' ENTERED AT 14:05:06 ON 12 JUN 2003
L9 3 S L7

FILE 'REGISTRY' ENTERED AT 14:06:05 ON 12 JUN 2003
L10 1 S 1225-58-7/RN

FILE 'CAPLUS' ENTERED AT 14:06:47 ON 12 JUN 2003
L11 17 S L10

FILE 'REGISTRY' ENTERED AT 14:08:46 ON 12 JUN 2003

FILE 'CAPLUS' ENTERED AT 14:08:57 ON 12 JUN 2003

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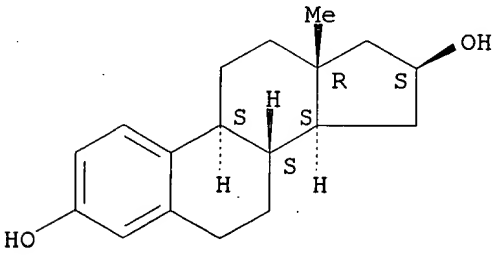
L11 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1987:16187 CAPLUS
DOCUMENT NUMBER: 106:16187
TITLE: Methylcholanthrene: a possible pseudosubstrate for adrenocortical 17.alpha.-hydroxylase and aryl hydrocarbon hydroxylase
AUTHOR(S): Hornsby, Peter J.; Aldern, Kathy A.; Harris, Sandra E.
CORPORATE SOURCE: Sch. Med., Univ. California, La Jolla, CA, 92093, USA
SOURCE: Biochemical Pharmacology (1986), 35(19), 3209-19
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **1225-58-7**, Estra-1,3,5(10)-triene-3,16.beta.-diol
RL: BIOL (Biological study)
(aryl hydrocarbon hydroxylase and steroid 17.alpha.-hydroxylase response to, in adrenocortical cells)
RN 1225-58-7 CAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

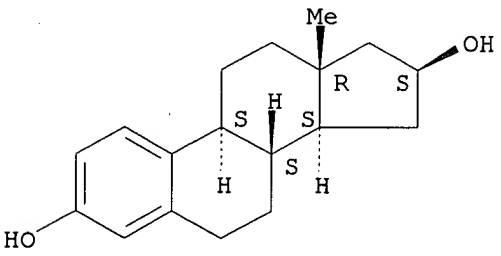


AB In cultured bovine adrenocortical cells, the loss of steroid 17.alpha.-hydroxylase (I) activity was obsd. after incubation with 3-methylcholanthrene (3-MC). The suppression of I by 3-MC was rapid (50% loss of activity in 10 h at 1 .mu.m 3-MC), did not exhibit a lag period, and was not affected by cycloheximide. Direct effects of 3-MC on I were obsd. only at high concns., but the concn. for 50% loss of activity was 0.3 .mu.M when 3-MC was added for 24 h prior to assay of I. High concns. (to 40 .mu.M) of substrate (progesterone), did not affect the loss of activity due to 3-MC. Loss of I activity was specific; steroid

11.beta.-hydroxylase was unaffected and cell growth was unaltered. However, 22-amino-23,24-bisnorchol-5-en-3.beta.-ol, an inhibitor of I, partially prevented the loss of I at 1-30 nM. 3-MC was thought to induce cytochrome P 450s via a receptor with high affinity for 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD). TCDD was without effect on I over the range 10 nM-10 .mu.M. Benz[a]anthracene, 7,12-dimethylbenz[a]anthracene, benzo[a]pyrene, chrysene, and methylphenanthrenes suppressed I at high concns. (10-50 .mu.M for 50% loss of activity). Some steroids that lack a substituent at position 17 also caused loss of I. Like I, bovine adrenocortical cell aryl hydrocarbon hydroxylase (II) was found to be suppressed by exposure to 3-MC. Compds. that caused loss of I caused loss of II, with a similar order of potency and at similar concns. Suppression of II by 3-MC did not require protein synthesis and was prevented by an inhibitor of enzymic activity, .alpha.-naphthoflavone. This implied a degree of similarity of the cytochrome P 450s for I and II, but the activities were shown to be likely due to different enzymes. The suppression of I and II by 3-MC appeared not to occur by a receptor-mediated mechanism but to be similar to the suppression of steroid 11.beta.-hydroxylase and steroid 21-hydroxylase by steroid pseudosubstrates previously obsd.

L11 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1985:574487 CAPLUS
DOCUMENT NUMBER: 103:174487
TITLE: Isolation of novel microbial 3.alpha.-, 3.beta.-, and 17.beta.-hydroxysteroid dehydrogenases. Purification, characterization, and analytical applications of a 17.beta.-hydroxysteroid dehydrogenase from an Alcaligenes sp
AUTHOR(S): Payne, Donna W.; Talalay, Paul
CORPORATE SOURCE: Sch. Med., Johns Hopkins Univ., Baltimore, MD, 21205, USA
SOURCE: Journal of Biological Chemistry (1985), 260(25), 13648-55
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **1225-58-7**
RL: BIOL (Biological study)
(17.beta.-hydroxy steroid dehydrogenase of Alcaligenes specificity for, structure in relation to)
RN 1225-58-7 CAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

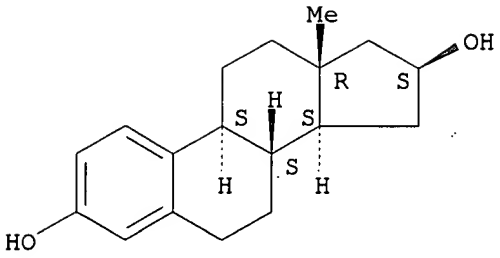


AB By selecting for growth on testosterone or 17.beta.-estradiol as the only source of org. C, a no. of soil microorganisms which contain highly active and novel, inducible, NAD-linked 3.alpha.-, 3.beta.-, and 17.beta.-hydroxy steroid dehydrogenases were isolated. Such enzymes are suitable for the microanal. of steroids and of steroid-transforming enzymes, as well as for performing stereoselective oxidns. and redn. of steroids. Of particular interest among these organisms is a new species of Alcaligenes contg. 17.beta.-hydroxy steroid dehydrogenase (I) easily separable from 3.beta.-hydroxy steroid dehydrogenase activity. Unlike any of the other isolated organisms, this Alcaligenes species contained no 3.alpha.-hydroxy steroid dehydrogenase activity. A large-scale purifn. (763-fold) to homogeneity of the major induced I was achieved by ion-exchange, hydrophobic, and affinity chromatogs. The enzyme has high specific activity for the oxidn. of testosterone (Vmax = 303 .mu.mol/min/mg protein; Km = 3.6 .mu.M) and reacts almost equally well with 17.beta.-estradiol (Vmax = 356 .mu.mol/min/mg; Km = 6.4 .mu.M). It consists of apparently identical subunits mol. wt. = 32,000) and exists in polymeric form under nondenaturing conditions (mol. wt. = 68,000 by gel filtration. and 86,000 by polyacrylamide gel electrophoresis). The isoelec. point is pH 5.1. The enzyme is almost completely specific for 17.beta.-hydroxy steroids which may be .DELTA.5-olefins or ring A phenols or have cis or trans A/B ring fusions. Substituents at other positions are tolerated, although the presence of a 16.alpha.- or 16.beta.-OH group blocks the oxidn. of the 17.beta.-OH function. 3.beta.-Hydroxy steroids (A/B ring fusion trans, but not cis, or .DELTA.5-olefins) are very poor substrates. The application of this highly active, specific, and stable I to the microestn. of steroids by enzymic cycling of nicotinamide nucleotides and for the stereospecific oxidn. of steroids is demonstrated.

L11 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1984:47664 CAPLUS
DOCUMENT NUMBER: 100:47664
TITLE: Inhibitor specificity of the placental microsomal oxidase system responsible for the aromatization of epitestosterone (17.alpha.-hydroxy-4-androsten-3-one)
AUTHOR(S): Sheean, Leon A.; Meigs, Robert A.
CORPORATE SOURCE: Sch. Med., Case Western Reserve Univ., Cleveland, OH, 44106, USA
SOURCE: Steroids (1983), 41(2), 225-41
CODEN: STEDAM; ISSN: 0039-128X
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **1225-58-7**
RL: BIOL (Biological study)
(epitestosterone oxidase of human placenta microsomes inhibition by)
RN 1225-58-7 CAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

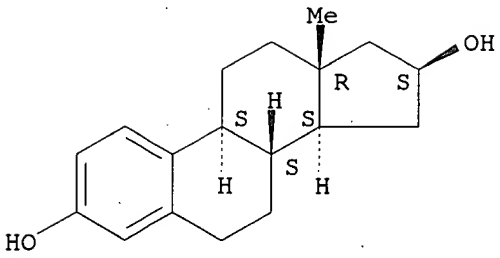
40997891



AB Human placental microsomes converted epitestosterone to 17.alpha.-estradiol at rates of 23-48 pmol/min/mg protein with a Km of 113 .mu.M. The activity was inhibited 70-90% by concns. of CO, metyrapone, octylamine, 7,8-benzoflavone, and 7-ethoxycoumarin which had no effect on the aromatization of 4-androstene-3,17-dione. Conversely, CN- and N3- were more effective inhibitors of the conversion of the latter androgen. A variety of neutral steroids inhibited the aromatization of epitestosterone with 19-norsteroids being particularly effective, but competitive effects could not be demonstrated. Both 17.beta.-hydroxy-4-estren-3-one and 16.alpha.-hydroxy-4-androstene-3,17-dione caused a mixed inhibition. A no. of phenolic steroids were also inhibitory with 16-oxo compds. being particularly effective. Inhibition by estrone was non-competitive (Ki = 16 .mu.M). The aromatization of epitestosterone resembles placental microsomal oxidase activities against estrone and benzo[a]pyrene in its inhibitor specificity and epitestosterone may be the native substrate for an oxidase also active in the metab. of arom. xenobiotic chems.

L11 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1981:561659 CAPLUS
DOCUMENT NUMBER: 95:161659
TITLE: Characteristics of membrane transport of methotrexate by cultured human breast cancer cells
AUTHOR(S): Schilsky, Richard L.; Bailey, Brenda D.; Chabner, Bruce A.
CORPORATE SOURCE: Div. Cancer Treat., Natl. Cancer Inst., Bethesda, MD, 20205, USA
SOURCE: Biochemical Pharmacology (1981), 30(12), 1537-42
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **1225-58-7**
RL: BIOL (Biological study)
(methotrexate transport by breast cancer cells response to)
RN 1225-58-7 CAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

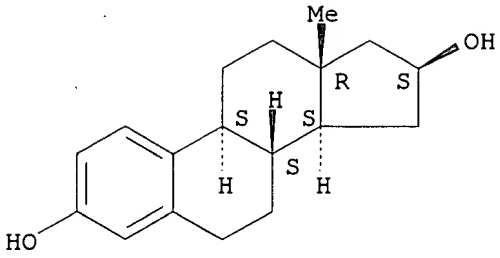
Absolute stereochemistry.



AB Methotrexate (I) [59-05-2] transport by MCF-7 cells and cultured estrogen- and insulin [9004-10-8]-sensitive human breast cancer cells exhibited a high-affinity carrier system that displayed Michaelis-Menten kinetics (Km 8.22.mu.M, Vmax 12.22 nmol/min/g cell protein), was competitively inhibited by leucovorin and aminopterin but not folic acid, and was temp.-sensitive (Q10 2.25). Initial uptake rates were not affected by ouabain or NaN3, but efflux of intracellular drug was markedly inhibited by NaN3, suggesting an energy-dependent efflux mechanism. A low affinity uptake component was identified with extracellular I >10.mu.M, possibly representing a lower affinity membrane carrier or passive diffusion. Growth of MCF-7 cells in serum-free medium induced an increase in Km to 15.93.mu.M; insulin, but not estradiol, reversed this change. Thus, I transport in this human solid tumor is similar to that in human leukemia cells.

L11 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1978:116912 CAPLUS
DOCUMENT NUMBER: 88:116912
TITLE: Inhibition of human placental 17.beta.-hydroxysteroid dehydrogenase by steroids and nonsteroidal alcohols: aspects of inhibitor structure and binding specificity
AUTHOR(S): Blomquist, Charles H.; Kotts, Claire E.; Hakanson, Erick Y.
CORPORATE SOURCE: Dep. Obstet. Gynecol., St. Paul-Ramsey Hosp., St. Paul, MN, USA
SOURCE: Archives of Biochemistry and Biophysics (1978), 186(1), 35-41
CODEN: ABBIA4; ISSN: 0003-9861
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **1225-58-7**
RL: BIOL (Biological study)
(17.beta.-hydroxysteroid dehydrogenase inhibition by, kinetics of)
RN 1225-58-7 CAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

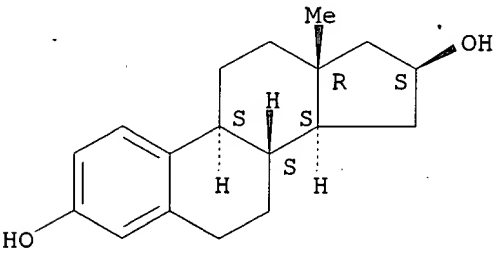
Absolute stereochemistry.

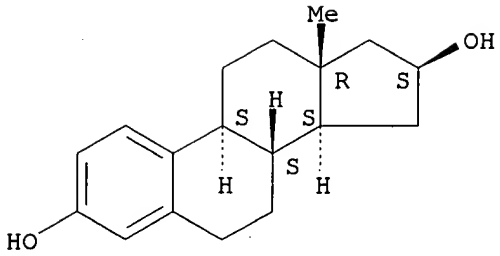


AB Inhibition of human placental 17.beta.-hydroxysteroid dehydrogenase by C18 and C19 steroids and nonsteroidal alcs. was assayed at pH 9.0 with 17.beta.-estradiol 3-Me ether and NAD as reactants. The nonsteroidal alcs. tested were poor inhibitors. Cyclopentanol and cyclohexanol had Ki values >5mM. Nonarom. C18 and C19 steroids with O functions at both positions 3 and 17 gave no detectable inhibition or had Ki values .gtoreq.160 .mu.m. 3.beta.-Hydroxy-5,16-androstadiene, 5-androsten-3.beta.-ol, 1,3,5(10)-estratrien-3-ol, and 1,3,5(10),16-estratetraen-3-ol, steroids lacking a C(17) oxygen function, had Ki values of 1.8, 6.0, 0.04, and 0.17 .mu.M, resp., demonstrating that both C18 and C19 steroids can bind at the steroid site. Binding specificity is narrowed and binding affinity for nonarom. steroids weakened by O functions at C(17) or both C(3) and C(17). The structural implications of the specificity data for steroid recognition and complex formation and in vivo control of enzyme activity are discussed.

L11 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1973:505459 CAPLUS
DOCUMENT NUMBER: 79:105459
TITLE: Chromogenic reactions of steroids with strong acids. IV. Specificity of the Kober reaction
AUTHOR(S): Kimura, Michiya; Kawata, Meiji; Akiyama, Kazuyuki; Harita, Kazuaki; Miura, Toshiaki
CORPORATE SOURCE: Fac. Pharm. Sci., Hokkaido Univ., Sapporo, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1973), 21(8), 1720-6
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **1225-58-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(Kober reaction of, absorption spectra and)
RN 1225-58-7 CAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

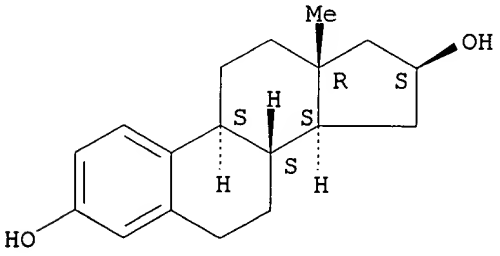




AB The structural requirements were investigated for the Kober reaction of steroidal mols. On the basis of the data given by 94 phenolic steroids and related substance, a compd. will give the pos. Kober reaction when a steroidal ring system, a phenolic ring A, double bond or O function in ring D, an angular Me group at C-13, and an angular H atom are present in its mol.

L11 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1970:495274 CAPLUS
DOCUMENT NUMBER: 73:95274
TITLE: Absorption and fluorescence spectra of phenolic steroids and their Kober chromophore
AUTHOR(S): De Lauzon, Solange
CORPORATE SOURCE: Lab. Chim. Biol., Fac. Med., Paris, Fr.
SOURCE: Bulletin de la Societe de Chimie Biologique (1970), 52(2), 181-209
CODEN: BSCIA3; ISSN: 0037-9042
DOCUMENT TYPE: Journal
LANGUAGE: French
IT **1225-58-7**
RL: PRP (Properties)
(fluorescence and visible spectra of, and its Kober chromogen)
RN 1225-58-7 CAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

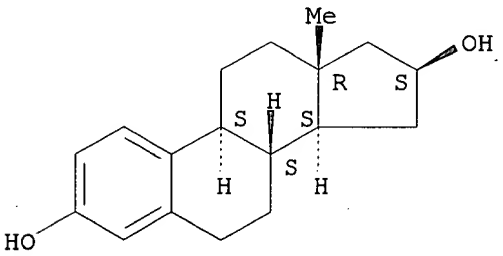


AB A complete assignment was made of the absorption and fluorescence spectra of a no. of phenolic steroids and their derivs. and the results may be used to identify and det. each estrogen studied. The reaction of various derivs. which cannot be differentiated by the behavior of the Kober chromophore, or do not form a Kober chromophore, in H2SO4 and H3PO4 was used as an identification method. These derivs. included ketonic derivs. of estrone and estradiol, 16-hydroxy derivs. of estrone and their Et and Me ethers, and non-oxygenated C17 derivs. The Kober reaction was used as

a detn. method for derivs. giving a characteristic absorption max., and the Ittrich modification allowed a sensitive anal. method to be developed for the steroid groups.

L11 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1970:452631 CAPLUS
DOCUMENT NUMBER: 73:52631
TITLE: Steroid utilization by amphibian skin
AUTHOR(S): Ferguson, M. M.; McGadey, J.
CORPORATE SOURCE: Anat. Dep., Univ. Glasgow, Glasgow, UK
SOURCE: Histochemie (1970), 22(1), 36-8
CODEN: HICHAU; ISSN: 0018-2222
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **1225-58-7**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(metabolism of, by skin)
RN 1225-58-7 CAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

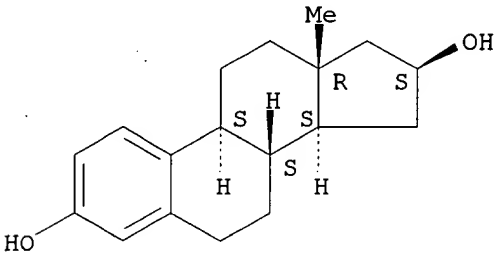


AB The glands which secrete unpleasant tasting or toxic substances in amphibian dermis were investigated histochem. for hydroxysteroid dehydrogenase (I) activity to draw comparisons with mammalian sebaceous glands, which are known to utilize hydroxy steroids. Skin sections from frogs were incubated with 15 different steroids; serial sections were also stained with hematoxylin and eosin and by the periodic acid-Schiff (PAS) reaction to differentiate mucous glands. The frog skin contained at least 2 functional types of glands; one type was PAS-pos., while the second type, less common, was PAS-neg. but exhibited intense I activity. Tissue incubated with pregnenolone, dehydroepiandrosterone, 3.beta.-hydroxyandrost-5-en-16-one 3-methyl ether, and 2.beta.-hydroxyprogesterone exhibited no formazan deposits.

L11 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1965:10380 CAPLUS
DOCUMENT NUMBER: 62:10380
ORIGINAL REFERENCE NO.: 62:1938e-f
TITLE: A search for inhibitors of prostate growth stimulators
AUTHOR(S): Tesar, Charles; Scott, William Wallace
CORPORATE SOURCE: Johns Hopkins Hosp., Baltimore, MD
SOURCE: Investigative Urology (1964), 1(5), 482-98
CODEN: INURAQ; ISSN: 0021-0005
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable
IT **1225-58-7**, Estra-1,3,5(10)-triene-3,16.beta.-diol
(as prostate growth inhibitor)
RN 1225-58-7 CAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

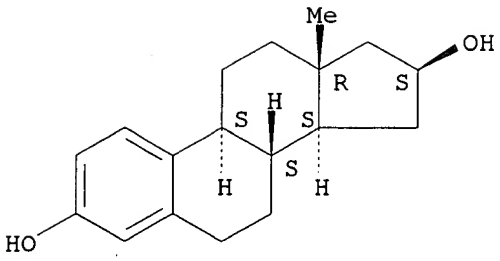
Absolute stereochemistry.



AB Wistar rats received 0.4 mg. testosterone propionate (I) subcutaneously every other day for 8 days following castration. Test compds. were given at 0.5, 1, and 2 mg. every other day for 7 days, with or without 0.4 mg. I in castrate and noncastrates, resp. Within 48 hrs. of the 7th (final) injection, animals were sacrificed with CHCl3, and the prostate wt. to body wt. ratio, and the prostate wt. index were detd. The greatest prostate growth inhibitor was 17.beta.-estradiol, and some weak inhibition was seen with 6.alpha.-methyl-4-pregnene-3,20-dione-17.alpha.-ol acetate, androstane-3,17-dione, and 2.alpha.-methyl-4-estren-17.beta.-ol-3-one, the inhibitory effect being seen only in intact rats, and not in castrates, for all 52 compds. tested.

L11 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1960:98911 CAPLUS
DOCUMENT NUMBER: 54:98911
ORIGINAL REFERENCE NO.: 54:18799c-d
TITLE: Cytostatic activities of steroidal estrogens against zebra-fish embryos
AUTHOR(S): Jones, Roy W.; Rhone, James R.; Huffman, Max N.
CORPORATE SOURCE: Oklahoma State Univ., Stillwater
SOURCE: Proceedings of the Society for Experimental Biology and Medicine (1960), 104, 190-1
CODEN: PSEBAA; ISSN: 0037-9727
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT **1225-58-7**, Estra-1,3,5(10)(triene-3,16.beta.-diol
(as cell-division inhibitor)
RN 1225-58-7 CAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

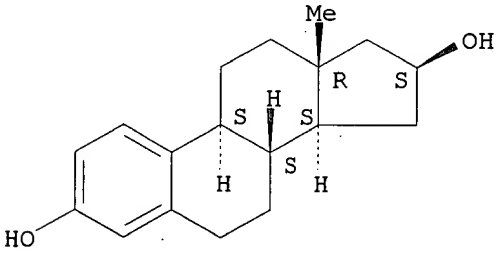
Absolute stereochemistry.



AB cf. CA 52, 3171c. The cytostatic effects of 14 steroidal estrogens (named) and the 3-Me and 3-Et ethers of each were tested on embryos of zebra-fish (Brachydanio rerio) as test object. Many were inactive in the concns. used. Most active was 17-dihydro-17 .beta.-equilin 3-ethyl ether (effective at 0.5 p.p.m.). There was no relation whatever between estrogenic hormone potency and cytostatic potency.

L11 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1959:17432 CAPLUS
DOCUMENT NUMBER: 53:17432
ORIGINAL REFERENCE NO.: 53:3276g-i,3277a-f
TITLE: Synthesis of 1,3,5(10)-estratriene-3,16.beta.,17.alpha.-triol
AUTHOR(S): Fishman, Jack; Biggerstaff, Warren R.
CORPORATE SOURCE: Sloan-Kettering Inst. for Cancer Research, New York, NY
SOURCE: Journal of Organic Chemistry (1958), 23, 1190-2
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT **1225-58-7**, Estra-1,3,5(10)(triene-3,16.beta.-diol (prepn. of)
RN 1225-58-7 CAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB Prepn. of 1,3,5(10)-estratriene-3,16.beta.,17.alpha.-triol (I) is described. The 16.alpha.- (II) and 16.alpha.-bromo epimers (III) of estrone were also prepd. and some of their reactions studied. Of the 4 possible estriols isomeric at C-16 and C-17 only 3 are known. The present authors undertook the prepn. of the remaining isomer, I. Estrone enol diacetate (1 g.) in CCl4 contg. some K2CO3 was treated with 1 equiv. of Br in CCl4 and the mixt. worked up to give 700 mg. 16.alpha.-bromoestrone acetate (IV), m. 169-71.degree. (MeOH), [.alpha.]24D 119.degree. (CHCl3).

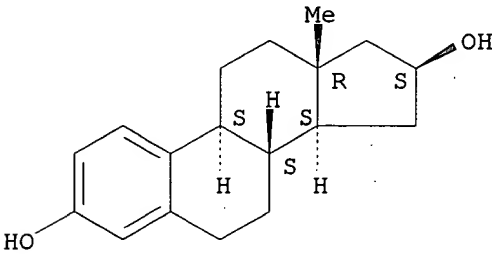
IV (0.3 g.) in 4% alc. H2SO4 left 20 hrs. at room temp., dild. with H2O, and extd. with CHCl3 gave 243 mg. II, needles, m. 225-8.degree. (C6H6), [.alpha.]24D 120.degree. (CHCl3). Acetylation of II with Ac2O and C5H5N regenerated IV. IV (0.5 g.) in a min. amt. of 1:1 C6H6-ligroine was absorbed on Al2O3, left overnight on the column and eluted with first 3:2 and then 4:1 C6H6-ligroine, and the fractions combined on the basis of m.p. The first 5 fractions gave on crystn. 0.23 g. pure IV. Fractions 6-10 were mixts., and fractions 10-14 gave 47 mg. 16.beta.-bromoestrone acetate (V), needles, m. 170-3.degree. (MeOH), [.alpha.]25D 156.degree. (CHCl3). Subsequent fractions eluted from the column with more polar solvents proved to be a mixt. of the hydrolyzed II and III. A mixed m.p. of V with IV showed a depression of 40.degree.; the infrared spectra of II and III in CS2 were different in the 1400-650 cm.-1, but there was no difference in the position of the CO band at 1758 cm.-1 Paper chromatography in several systems failed to sep. the 2 isomers. Room temp. hydrolysis of V 20 hrs. with 4% alc. H2SO4 gave free III, needles, m. 224-7.degree. (sublimation) (C6H6). An analytical sample of III m. 225-8.degree., [.alpha.]24D 154.degree. (CHCl3). III could be obtained by refluxing IV with 4% alc. H2SO4 overnight; the resultant mixt. was predominantly III which was purified by fractional crystn. Acetylation of III gave V. IV (1 g.) stirred 2 hrs. at 0.degree. with excess LiAlH4 in anhyd. Et2O, the excess reagent destroyed with H2O and acidified with dil. HCl, and the org. phase evapd. gave 0.78 g. gum. Without purification, the material refluxed 4 hrs. with 5% alc. KOH, dild. with H2O, extd. with CHCl3, and chromatographed on Al2O3 gave 0.24 g. 16.beta.,17.beta.-epoxy-1,3,5(10)-estratrien-3-ol (VI), m. 200-4.degree. (C6H6-ligroine), [.alpha.]25D 119.degree. (CHCl3), and 92 mg. estrone. The structure of VI was established by reduction with LiAlH4 to give 16.beta.-estradiol (VII), identical with a specimen prepd. from 1,3,5(10)-estratrien-16-one by NaBH4 reduction. VII m. 224-6.degree.. V (150 mg.) reduced under identical conditions with LiAlH4 followed by heating with alkali gave 94 mg. estrone. No 16.alpha.,17.alpha.-oxide was isolated. VI (0.3 g.) in 30 cc. AcOH refluxed 4 hrs., evapd., refluxed 1.5 hrs. with 6% alc. KOH, dild., acidified, and extd. with CHCl3 gave 0.3 g. solid which was chromatographed on Al2O3 to give 124 mg. I, m. 248-50.degree. (C6H6-MeOH), [.alpha.]25D 61.degree. (alc.). The subsequent fractions eluted weighed 64 mg. and proved to be the other trans isomer, 1,3,5(10)-estratriene-3,16.beta.,17.alpha.-triol (VIII). The infrared spectrum of I in KBr showed differences from the other 3 estriol isomers. Paper chromatography in C6H6-MeOH-H2O-EtOAc system sepd. I from its isomers. I was less polar than VIII but considerably more polar than the 2 cis triols in the solvent system used. 1,3,5(10),16-Estratetraen-3-ol benzoate (100 mg.), m. 161-6.degree., in Et2O treated with BzO2H gave 111 mg. crude 16.alpha.,17.alpha.-epoxy-1,3,5(10)-estratrien-3-ol benzoate. Without further purification this material was refluxed 2 hrs. with 3 cc. AcOH under N, the AcOH removed, and the residue refluxed 1.5 hrs. in 8% alc. KOH to give 73 mg. yellow solid, which, decolorized and crystd., gave 23 mg. solid which was chromatographed on silica to give 12 mg. I. These results confirm the assignment of the Br orientation in II and III and also support the previous finding (C.A. 52, 5445b) that a 16.beta.-substituent results in the stereospecific .beta.-reduction of the 17-one while a 16.alpha.-substituent makes the reduction only stereoselective, with about 10-15% of .alpha.-reduction. The pharmacol. effects are being investigated.

L11 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1958:93818 CAPLUS

40997891

DOCUMENT NUMBER: 52:93818
ORIGINAL REFERENCE NO.: 52:16548d-f
TITLE: Comparative ability of some steroids and their esters to enhance the renal .beta.-glucuronidase activity of mice
AUTHOR(S): Fishman, Wm. H.; Lipkind, J. B.
CORPORATE SOURCE: Tufts Univ. School of Med., Boston, MA
SOURCE: Journal of Biological Chemistry (1958), 232, 729-36
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT **1225-58-7**, Estra-1,3,5(10)(triene-3,16.beta.-diol
(potentiation of .beta.-glucuronidase of kidneys by)
RN 1225-58-7 CAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

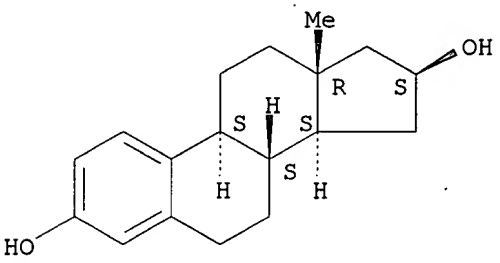


AB cf. C.A. 50, 17081h. The mouse renal .beta.-glucuronidase response permits a more reliable estimate of the potency of testosterone esters. A dose-response curve in which greatly reduced amts. of steroid were used was employed. The potency of a steroid in eliciting the .beta.-glucuronidase response is defined as 24 times the reciprocal of the dose required to produce a kidney assaying 10,000 units/g. The standard of reference is testosterone. According to this measure, testosterone propionate shows a potency of 60 and that of testosterone is 3.0. Nortestosterone cyclopentylpropionate was the most potent compd. (potency 150). There is a marked difference in response between testosterone propionate and its other esters vs. testosterone. 3,16.beta.-Estradiol and 16-oxoestrone gave 2- to 3-fold increases in renal .beta.-glucuronidase. The introduction of a 17-Me or 17-Et group into nortestosterone increased its potency as detd. by the renal .beta.-glucuronidase response.

L11 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1957:101244 CAPLUS
DOCUMENT NUMBER: 51:101244
ORIGINAL REFERENCE NO.: 51:18311d-g
TITLE: The effect of natural and synthetic estrogens on reticuloendothelial system function
AUTHOR(S): Heller, J. H.; Meier, R. M.; Zucker, R.; Mast, G. W.
CORPORATE SOURCE: New England Inst. for Med. Research, Ridgefield, CT
SOURCE: Endocrinology (1957), 61, 235-41
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT **1225-58-7**, Estra-1,3,5(10)(triene-3,16.beta.-diol

(effect on reticuloendothelial system)
RN 1225-58-7 CAPLUS
CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB The activity of the reticuloendothelial system was detd. by measuring the rate of disappearance by phagocytosis of intravenously injected colloidal C from the blood. The colloid uptake of various organs was detd. by assaying for CrP3204 content after an intravenous injection. Steroids increasing phagocytic velocity 100% or more were: estradiol, ethynylestradiol, estradiol-16-one, 1,3,5-estratriene-3,16.beta.-diol, 3-methoxy-1,3,5-estratriene-16.beta.-ol, estriol, 16-epiestriol, 3-methoxy-1,3,5-estratriene-16.beta.,17.beta.-diol, and 3-ethoxy-1,3,5-estratriene-16.beta.,17.beta.-diol; inactive were: 5-androstene-3.beta.,16.beta.-diol, androstane-3,16.beta.-diol, androstane-3.alpha.-ol-16-one, 4-androstene-3,16-dione, 5-androstene-3.beta.-ol-16-one, 3.beta.-methoxy-5-androstene-16-one, 1,3,5-estratriene-3,6.alpha.-diol, and 3-methoxy-1,3,5-estratriene-16-one. Stimulated activity of the reticuloendothelial system was accompanied by liver and spleen enlargement, without however, much increase in total colloid uptake by these organs.

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	60.64	151.86

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-8.46	-16.91

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DICTIONARY FILE UPDATES: 11 JUN 2003 HIGHEST RN 529474-19-9

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http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> s Estra-1,3,5(10)-triene-3,16-diol, 7-alkyl
MISSING OPERATOR 'STRA-1,3,5(10'

=> s Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl
MISSING OPERATOR 'STRA-1,3,5(10'

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.40	152.26

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CA SUBSCRIBER PRICE	0.00	-16.91

FILE 'CAPLUS' ENTERED AT 14:12:14 ON 12 JUN 2003
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FILE COVERS 1907 - 12 Jun 2003 VOL 138 ISS 24
FILE LAST UPDATED: 11 Jun 2003 (20030611/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl
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The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> s Estra-1,3,5(10)-triene-3,16-diol,7-ethyl
MISSING OPERATOR 'STRA-1,3,5(10'
The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00     -16.91

FILE 'REGISTRY' ENTERED AT 14:13:03 ON 12 JUN 2003
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STRUCTURE FILE UPDATES:   11 JUN 2003  HIGHEST RN 529474-19-9
DICTIONARY FILE UPDATES:  11 JUN 2003  HIGHEST RN 529474-19-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.80     153.48

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00     -16.91

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STRUCTURE FILE UPDATES:   11 JUN 2003  HIGHEST RN 529474-19-9
DICTIONARY FILE UPDATES:  11 JUN 2003  HIGHEST RN 529474-19-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.
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Crossover limits have been increased. See HELP CROSSOVER for details.

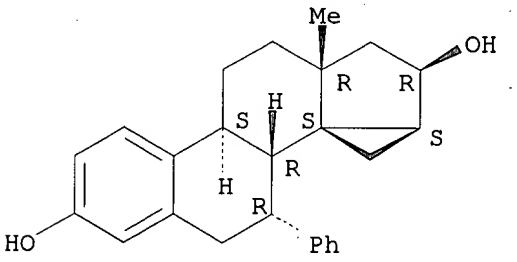
Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> s 287723-43-7/rn
L12 1 287723-43-7/RN

=> d l12

L12 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS
RN **287723-43-7** REGISTRY
CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol, 3',15-dihydro-7-phenyl-, (7.alpha.,14S,15.alpha.,16.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H28 O2
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.08	155.56

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-16.91

FILE 'CAPLUS' ENTERED AT 14:14:48 ON 12 JUN 2003
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FILE COVERS 1907 - 12 Jun 2003 VOL 138 ISS 24
FILE LAST UPDATED: 11 Jun 2003 (20030611/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 13:10:32 ON 12 JUN 2003)

FILE 'REGISTRY' ENTERED AT 13:10:38 ON 12 JUN 2003
L1 1 S 28834-40-4/RN
L2 1 S L1 FULL

FILE 'CAPLUS' ENTERED AT 13:12:23 ON 12 JUN 2003
L3 3 S L2

FILE 'REGISTRY' ENTERED AT 13:17:42 ON 12 JUN 2003
L4 STR 28834-40-4
L5 0 S L4 FAM SAM

FILE 'REGISTRY' ENTERED AT 14:03:13 ON 12 JUN 2003
L6 1 S 16 ALPHA ESTRADIOL

FILE 'CAPLUS' ENTERED AT 14:03:51 ON 12 JUN 2003
L7 3 S L1

FILE 'REGISTRY' ENTERED AT 14:04:32 ON 12 JUN 2003
L8 1 S 1090-04-6/RN

FILE 'CAPLUS' ENTERED AT 14:05:06 ON 12 JUN 2003
L9 3 S L7

FILE 'REGISTRY' ENTERED AT 14:06:05 ON 12 JUN 2003
L10 1 S 1225-58-7/RN

FILE 'CAPLUS' ENTERED AT 14:06:47 ON 12 JUN 2003
L11 17 S L10

FILE 'REGISTRY' ENTERED AT 14:08:46 ON 12 JUN 2003

FILE 'CAPLUS' ENTERED AT 14:08:57 ON 12 JUN 2003

FILE 'REGISTRY' ENTERED AT 14:11:21 ON 12 JUN 2003

FILE 'CAPLUS' ENTERED AT 14:12:14 ON 12 JUN 2003

FILE 'REGISTRY' ENTERED AT 14:13:03 ON 12 JUN 2003

FILE 'REGISTRY' ENTERED AT 14:14:16 ON 12 JUN 2003
L12 1 S 287723-43-7/RN

FILE 'CAPLUS' ENTERED AT 14:14:48 ON 12 JUN 2003

=> s l12 full
L13 1 L12

=> d l13 ibib hitstr abs

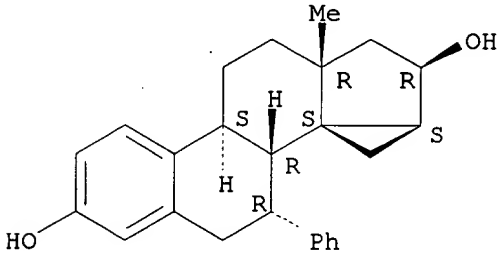
L13 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:552017 CAPLUS
DOCUMENT NUMBER: 133:150782
TITLE: synthesis of 16-Hydroxyestratrienes as selectively effective estrogens
INVENTOR(S): Kuenzer, Hermann; Knauthe, Rudolf; Lessl, Monika; Fritzemeier, Karl-heinrich; Hegele-Hartung, Christa; Boemer, Ulf; Mueller, Gerd; Kosemund, Dirk
PATENT ASSIGNEE(S): Schering A.-G., Germany
SOURCE: Ger. Offen., 34 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19906159	A1	20000810	DE 1999-19906159	19990209
CA 2359660	AA	20000817	CA 2000-2359660	20000209
WO 2000047603	A2	20000817	WO 2000-EP1073	20000209
WO 2000047603	A3	20010802		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2000029095	A5	20000829	AU 2000-29095	20000209
EP 1144431	A2	20011017	EP 2000-907539	20000209
EP 1144431	A3	20020612		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000008076	A	20020205	BR 2000-8076	20000209
JP 2002536455	T2	20021029	JP 2000-598520	20000209
EE 200100412	A	20021216	EE 2001-412	20000209
NO 2001003860	A	20011008	NO 2001-3860	20010808
BG 105804	A	20020329	BG 2001-105804	20010809

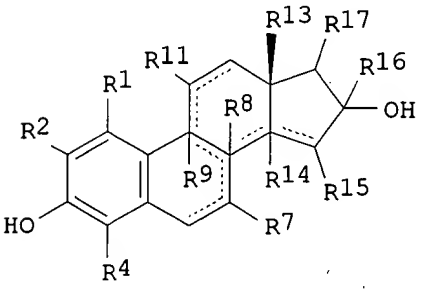
PRIORITY APPLN. INFO.: DE 1999-19906159 A 19990209
WO 2000-EP1073 W 20000209
OTHER SOURCE(S): MARPAT 133:150782

IT **287723-43-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of 16-Hydroxyestratrienes as selectively effective estrogens)
RN 287723-43-7 CAPLUS
CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol, 3',15-dihydro-7-phenyl-, (7.alpha.,14S,15.alpha.,16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



GI



I

AB Synthesis of 16-Hydroxyestratrienes (I) [R1 = halogen, HO, Me, F3C, MeO, EtO, H; R2 = halogen, HO, (un)substituted alkoxy, H; R4 = halogen, fluoroalkyl, F3C, F5C2, (un)substituted alkoxy, H; R7 = halogen, (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkoxy, (un)substituted heteroaryl, (un)substituted aryl, H; R8 = H, fluoroalkyl, fluoroalkenyl, CN; R9 = H, Me, Et, F3C, F5C2; R11 = NO2O, HO, HS, halogen, chloromethyl, fluoroalkenyl, fluoroalkyl, (un)substituted alkoxy, (un)substituted alkylthio, (un)substituted aryl, (un)substituted heteroaryl, H; R13 = Me, Et, F3C, F5C2; R14 = (un)substituted alkenyl, (un)substituted alkyl, H; R15 = halogen, fluoroalkyl, fluoroalkenyl, =O, =S, SO, SO2, (un)substituted =NH; R14, R15 together = methylene; R16 = fluoroalkyl, fluoroalkenyl, F3C, F5C2,CN, H; R17 = fluoroalkyl, fluoroalkenyl, H, HO] as selectively effective estrogens is disclosed. Thus, 16.alpha.-estradiol shows a 50% uterine stimulation at 30 .upsilon.g in in vivo testing.

=> logoff

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ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
LOGOFF? (Y)/N/HOLD:H

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	5.79	161.35

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.65	-17.56

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 14:16:29 ON 12 JUN 2003

BR 6914715	A0	19730524	BR 1969-214715	19691203
FR 2032446	A5	19701127	FR 1970-3091	19700129
FR 2032446	B1	19730713		
US 3660435	A	19720502	US 1970-10648	19700211
GB 1246944	A	19710922	GB 1970-1246944	19700212
CS 163204	P	19750829	CS 1970-995	19700212
CS 163205	P	19750829	CS 1970-3137	19700212
SE 372937	B	19750120	SE 1970-2170	19700220
ES 376888	A1	19720516	ES 1970-376888	19700225
PL 71511	P	19740629	PL 1970-138993	19700225
BE 746546	A	19700826	BE 1970-746546	19700226
NL 7002749	A	19700831	NL 1970-2749	19700226
AT 295055	B	19711227	AT 1970-1789	19700226
AT 298699	B	19720525	AT 1970-9356	19700226
DK 124540	B	19721030	DK 1970-950	19700226
JP 52015593	B4	19770430	JP 1970-16337	19700227
DK 128495	B	19740513	DK 1971-2950	19710616

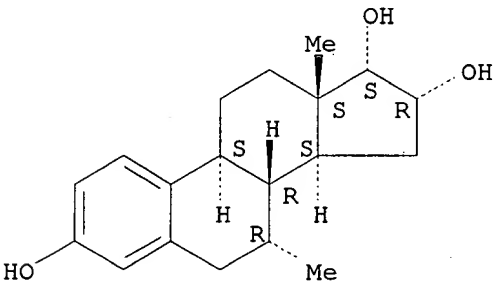
PRIORITY APPLN. INFO.: CH 1969-2962 19690227

IT **28834-40-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 28834-40-4 CAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, 7-methyl-, (7.alpha.,16.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



GI For diagram(s), see printed CA Issue.

AB The estrogenic, antigonadotropic, ovulation inhibiting, and (or) blastocyte implantation inhibiting title compd. (I) was prepd. by the treatment of II (prepd. from 7.alpha.-methylestrone by known methods) with OsO4 in pyridine at room temp. in the dark followed by refluxing with NaHSO3 in EtOH. I was also prepd. by the redn. of III with LiAlH4 in refluxing THF.

=>
=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	14.44	69.34
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.95	-5.85

FILE COVERS 1907 - 12 Jun 2003 VOL 138 ISS 24
FILE LAST UPDATED: 11 Jun 2003 (20030611/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> s l7
L9            3 L1

=> d his

     (FILE 'HOME' ENTERED AT 13:10:32 ON 12 JUN 2003)

     FILE 'REGISTRY' ENTERED AT 13:10:38 ON 12 JUN 2003
L1            1 S 28834-40-4/RN
L2            1 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 13:12:23 ON 12 JUN 2003
L3            3 S L2

     FILE 'REGISTRY' ENTERED AT 13:17:42 ON 12 JUN 2003
L4              STR 28834-40-4
L5            0 S L4 FAM SAM

     FILE 'REGISTRY' ENTERED AT 14:03:13 ON 12 JUN 2003
L6            1 S 16 ALPHA ESTRADIOL

     FILE 'CAPLUS' ENTERED AT 14:03:51 ON 12 JUN 2003
L7            3 S L1

     FILE 'REGISTRY' ENTERED AT 14:04:32 ON 12 JUN 2003
L8            1 S 1090-04-6/RN

     FILE 'CAPLUS' ENTERED AT 14:05:06 ON 12 JUN 2003
L9            3 S L7

=> d l9 1-3 ibib hitstr abs

L9   ANSWER 1 OF 3  CAPLUS  COPYRIGHT 2003 ACS
ACCESSION NUMBER:         1973:537384  CAPLUS
DOCUMENT NUMBER:          79:137384
TITLE:                    Highly active estratriols
INVENTOR(S):              Anner, Georg; Kalvoda, Jaroslav
```

40997891

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2209244	A	19720921	DE 1972-2209244	19720226
ZA 7201169	A	19721129	ZA 1972-1169	19720222
BE 780172	A1	19720904	BE 1972-114642	19720303
NL 7202873	A	19720907	NL 1972-2873	19720303
FR 2128593	A5	19721020	FR 1972-7489	19720303

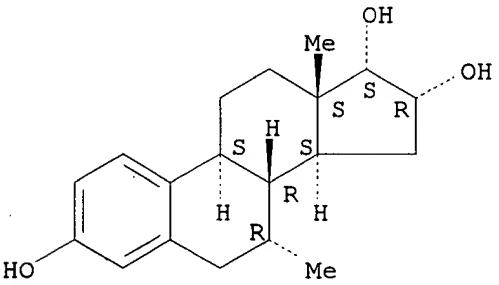
PRIORITY APPLN. INFO.: CH 1971-3234 19710305

IT **28834-40-4**
RL: BIOL (Biological study)
(pharmaceutical, for menopause disorder treatment)

RN 28834-40-4 CAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, 7-methyl-, (7.alpha.,16.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB Formulations contg. tranquilizing 9-(methylaminomethyl)-9,10-dihydro-9,10-ethanoanthracene (I) in addn. to an estrogen, useful against climacteric irritations, were described. A typical tablet contained I 5.0, 7.alpha.-methylestrone 0.2, lactose 88.0, wheat starch 45.8, colloidal silicic acid 5.0, talc 5.0, and Mg stearate 1.0 mg.

L9 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1970:509986 CAPLUS
DOCUMENT NUMBER: 73:109986
TITLE: 7.alpha.-Methyl-3,16.alpha.,17.beta.-trihydroxyestra-1,3,5(10)-triene
INVENTOR(S): Anner, Georg; Kalvoda, Jaroslav
PATENT ASSIGNEE(S): CIBA Ltd.
SOURCE: Ger. Offen., 14 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2007416	A	19700910	DE 1970-2007416	19700218
DE 2007416	C3	19730517		
CH 537914	A	19730731	CH 1969-2962	19690227

40997891

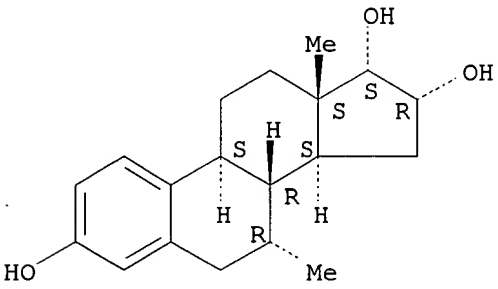
PATENT ASSIGNEE(S): Civa-Geigy A.-G.
SOURCE: Patentschrift (Switz.), 3 pp.
CODEN: SWXXAS
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 538460	A	19730815	CH 1973-3101	19690227

PRIORITY APPLN. INFO.: CH 1973-3101 19690227

IT **28834-40-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); IMF (Industrial manufacture); BIOL (Biological study); PREP (Preparation)
(manuf. and biol. activity of)
RN 28834-40-4 CAPLUS
CN Estra-1,3,5(10)-triene-3,16,17-triol, 7-methyl-, (7.alpha.,16.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



GI For diagram(s), see printed CA Issue.
AB Estratrienetriol I (R = R3 = H; R1 = R2 = OH) (II) was prepd. from 7.alpha.-methylestrone (I, RR1 = O, R2 = R3 = H). Thus, I (RR1 = O, R2 = R3 = H) was treated with CH2:C(OAc)Me and the product III was epoxidized to I (R = H, R1R2 = O, R3 = Ac). LiAlH4 redn. of the latter and subsequent hydrolysis gave II. II had estrogenic activity in Allen-Doisy test of 0.001-0.1 mg/kg s.c. and 0.02-0.3 mg/kg orally in rats, and in Buelbring-Buen test of 0.0003-0.003 mg/kg s.c. and 0.003-0.03 mg/kg orally in rats. II had antigonadotropic activity of 0.0003-0.003 mg/kg s.c. or 0.003-0.01 mg/kg orally in Parabiosis test. Also, II inhibited ovulation and embryo implantation.

L9 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1972:568615 CAPLUS
DOCUMENT NUMBER: 77:168615
TITLE: Menopausal hormone compositions
INVENTOR(S): Desaulles, Pierre A.; Hunger, Alfred; Bein, Hugo J.
PATENT ASSIGNEE(S): Ciba-Geigy A.-G.
SOURCE: Ger. Offen., 21 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German

40997891

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NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	Jun 03	New e-mail delivery for search results now available
NEWS 4	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 5	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS 6	Aug 26	Sequence searching in REGISTRY enhanced
NEWS 7	Sep 03	JAPIO has been reloaded and enhanced
NEWS 8	Sep 16	Experimental properties added to the REGISTRY file
NEWS 9	Sep 16	CA Section Thesaurus available in CAPLUS and CA
NEWS 10	Oct 01	CASREACT Enriched with Reactions from 1907 to 1985
NEWS 11	Oct 24	BEILSTEIN adds new search fields
NEWS 12	Oct 24	Nutraceuticals International (NUTRACEUT) now available on STN
NEWS 13	Nov 18	DKILIT has been renamed APOLLIT
NEWS 14	Nov 25	More calculated properties added to REGISTRY
NEWS 15	Dec 04	CSA files on STN
NEWS 16	Dec 17	PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS 17	Dec 17	TOXCENTER enhanced with additional content
NEWS 18	Dec 17	Adis Clinical Trials Insight now available on STN
NEWS 19	Jan 29	Simultaneous left and right truncation added to COMPENDEX, ENERGY, INSPEC
NEWS 20	Feb 13	CANCERLIT is no longer being updated
NEWS 21	Feb 24	METADEX enhancements
NEWS 22	Feb 24	PCTGEN now available on STN
NEWS 23	Feb 24	TEMA now available on STN
NEWS 24	Feb 26	NTIS now allows simultaneous left and right truncation
NEWS 25	Feb 26	PCTFULL now contains images
NEWS 26	Mar 04	SDI PACKAGE for monthly delivery of multifile SDI results
NEWS 27	Mar 20	EVENTLINE will be removed from STN
NEWS 28	Mar 24	PATDPAFULL now available on STN
NEWS 29	Mar 24	Additional information for trade-named substances without structures available in REGISTRY
NEWS 30	Apr 11	Display formats in DGENE enhanced
NEWS 31	Apr 14	MEDLINE Reload
NEWS 32	Apr 17	Polymer searching in REGISTRY enhanced
NEWS 33	Apr 21	Indexing from 1947 to 1956 being added to records in CA/CAPLUS
NEWS 34	Apr 21	New current-awareness alert (SDI) frequency in WPIDS/WPINDEX/WPIX
NEWS 35	Apr 28	RDISCLOSURE now available on STN
NEWS 36	May 05	Pharmacokinetic information and systematic chemical names added to PHAR
NEWS 37	May 15	MEDLINE file segment of TOXCENTER reloaded
NEWS 38	May 15	Supporter information for ENCOMPPAT and ENCOMPLIT updated
NEWS 39	May 16	CHEMREACT will be removed from STN

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 NEWS 40   May 19  Simultaneous left and right truncation added to WSCA
 NEWS 41   May 19  RAPRA enhanced with new search field, simultaneous left and
                   right truncation
 NEWS 42   Jun 06  Simultaneous left and right truncation added to CBNB
 NEWS 43   Jun 06  PASCAL enhanced with additional data

 NEWS EXPRESS  April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT
               MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
               AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

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  * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 13:10:32 ON 12 JUN 2003

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.21       0.21

FILE 'REGISTRY' ENTERED AT 13:10:38 ON 12 JUN 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   11 JUN 2003  HIGHEST RN 529474-19-9
DICTIONARY FILE UPDATES:  11 JUN 2003  HIGHEST RN 529474-19-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> s 28834-40-4/rn
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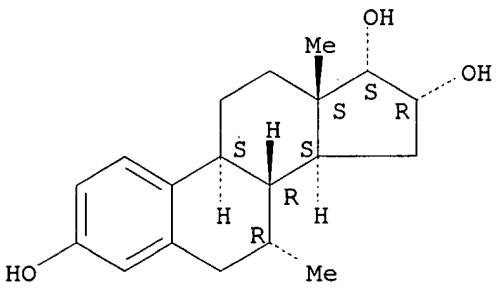
L1 1 28834-40-4/RN

=> d l1

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS
RN **28834-40-4** REGISTRY
CN Estra-1,3,5(10)-triene-3,16,17-triol, 7-methyl-,
(7.alpha.,16.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estra-1,3,5(10)-triene-3,16.alpha.,17.alpha.-triol, 7.alpha.-methyl- (8CI)
OTHER NAMES:
CN 7.alpha.-Methyl-3,16.alpha.,17.alpha.-trihydroxy-.DELTA.1,3,5(10)-
estratriene
CN 7.alpha.-Methylestra-1,3,5(10)-triene-3,16.alpha.,17.alpha.-triol
FS STEREOSEARCH
MF C19 H26 O3
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1957 TO DATE)
3 REFERENCES IN FILE CAPLUS (1957 TO DATE)

=> s l1 full
L2 1 28834-40-4/RN

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.88	3.09

FILE 'CAPLUS' ENTERED AT 13:12:23 ON 12 JUN 2003

FILE COVERS 1907 - 12 Jun 2003 VOL 138 ISS 24
FILE LAST UPDATED: 11 Jun 2003 (20030611/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l2
L3 3 L2

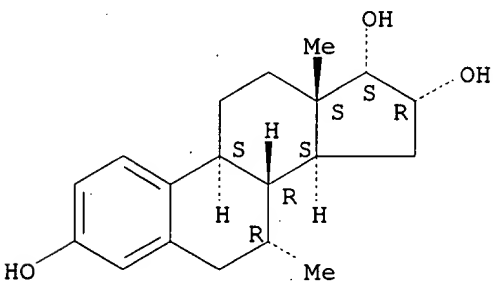
=> d l3 ibib hitstr abs

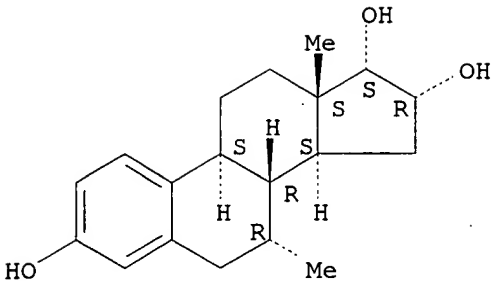
L3 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1973:537384 CAPLUS
DOCUMENT NUMBER: 79:137384
TITLE: Highly active estratriols
INVENTOR(S): Anner, Georg; Kalvoda, Jaroslav
PATENT ASSIGNEE(S): Civa-Geigy A.-G.
SOURCE: Patentschrift (Switz.), 3 pp.
CODEN: SWXXAS
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 538460	A	19730815	CH 1973-3101	19690227

PRIORITY APPLN. INFO.: CH 1973-3101 19690227
IT **28834-40-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); IMF (Industrial manufacture); BIOL (Biological study); PREP (Preparation)
(manuf. and biol. activity of)
RN 28834-40-4 CAPLUS
CN Estra-1,3,5(10)-triene-3,16,17-triol, 7-methyl-, (7.alpha.,16.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





GI For diagram(s), see printed CA Issue.

AB Estratrienetriol I (R = R3 = H; R1 = R2 = OH) (II) was prepd. from 7.alpha.-methylestrone (I, RR1 = O, R2 = R3 = H). Thus, I (RR1 = O, R2 = R3 = H) was treated with CH2:C(OAc)Me and the product III was epoxidized to I (R = H, R1R2 = O, R3 = Ac). LiAlH4 redn. of the latter and subsequent hydrolysis gave II. II had estrogenic activity in Allen-Doisy test of 0.001-0.1 mg/kg s.c. and 0.02-0.3 mg/kg orally in rats, and in Buelbring-Buen test of 0.0003-0.003 mg/kg s.c. and 0.003-0.03 mg/kg orally in rats. II had antigonadotropic activity of 0.0003-0.003 mg/kg s.c. or 0.003-0.01 mg/kg orally in Parabiosis test. Also, II inhibited ovulation and embryo implantation.

=> d his

(FILE 'HOME' ENTERED AT 13:10:32 ON 12 JUN 2003)

FILE 'REGISTRY' ENTERED AT 13:10:38 ON 12 JUN 2003
L1 1 S 28834-40-4/RN
L2 1 S L1 FULL

FILE 'CAPLUS' ENTERED AT 13:12:23 ON 12 JUN 2003
L3 3 S L2

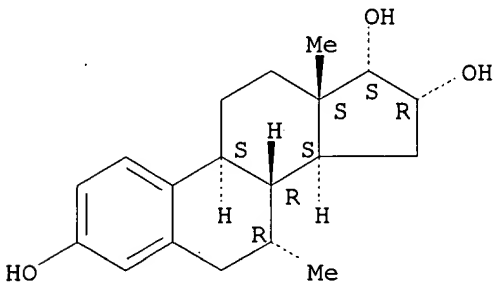
=> d l3 2-3 ibib hitstr abs

L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1972:568615 CAPLUS
DOCUMENT NUMBER: 77:168615
TITLE: Menopausal hormone compositions
INVENTOR(S): Desaulles, Pierre A.; Hunger, Alfred; Bein, Hugo J.
PATENT ASSIGNEE(S): Ciba-Geigy A.-G.
SOURCE: Ger. Offen., 21 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2209244	A	19720921	DE 1972-2209244	19720226
ZA 7201169	A	19721129	ZA 1972-1169	19720222
BE 780172	A1	19720904	BE 1972-114642	19720303
NL 7202873	A	19720907	NL 1972-2873	19720303

FR 2128593 A5 19721020 FR 1972-7489 19720303
PRIORITY APPLN. INFO.: CH 1971-3234 19710305
IT **28834-40-4**
RL: BIOL (Biological study)
(pharmaceutical, for menopause disorder treatment)
RN 28834-40-4 CAPLUS
CN Estra-1,3,5(10)-triene-3,16,17-triol, 7-methyl-,
(7.alpha.,16.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB Formulations contg. tranquilizing 9-(methylaminomethyl)-9,10-dihydro-9,10-ethanoanthracene (I) in addn. to an estrogen, useful against climacteric irritations, were described. A typical tablet contained I 5.0, 7.alpha.-methylestrone 0.2, lactose 88.0, wheat starch 45.8, colloidal silicic acid 5.0, talc 5.0, and Mg stearate 1.0 mg.

L3 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1970:509986 CAPLUS
DOCUMENT NUMBER: 73:109986
TITLE: 7.alpha.-Methyl-3,16.alpha.,17.beta.-trihydroxyestra-1,3,5(10)-triene
INVENTOR(S): Anner, Georg; Kalvoda, Jaroslav
PATENT ASSIGNEE(S): CIBA Ltd.
SOURCE: Ger. Offen., 14 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2007416	A	19700910	DE 1970-2007416	19700218
DE 2007416	C3	19730517		
CH 537914	A	19730731	CH 1969-2962	19690227
BR 6914715	A0	19730524	BR 1969-214715	19691203
FR 2032446	A5	19701127	FR 1970-3091	19700129
FR 2032446	B1	19730713		
US 3660435	A	19720502	US 1970-10648	19700211
GB 1246944	A	19710922	GB 1970-1246944	19700212
CS 163204	P	19750829	CS 1970-995	19700212
CS 163205	P	19750829	CS 1970-3137	19700212
SE 372937	B	19750120	SE 1970-2170	19700220
ES 376888	A1	19720516	ES 1970-376888	19700225

PL 71511	P	19740629	PL 1970-138993	19700225
BE 746546	A	19700826	BE 1970-746546	19700226
NL 7002749	A	19700831	NL 1970-2749	19700226
AT 295055	B	19711227	AT 1970-1789	19700226
AT 298699	B	19720525	AT 1970-9356	19700226
DK 124540	B	19721030	DK 1970-950	19700226
JP 52015593	B4	19770430	JP 1970-16337	19700227
DK 128495	B	19740513	DK 1971-2950	19710616

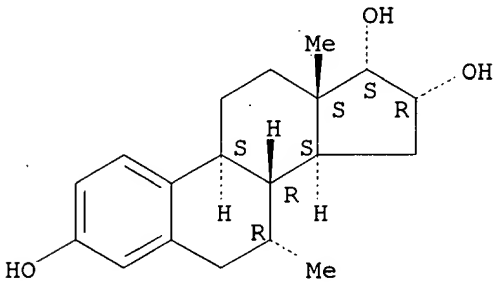
PRIORITY APPLN. INFO.: CH 1969-2962 19690227

IT **28834-40-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 28834-40-4 CAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, 7-methyl-, (7.alpha.,16.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



GI For diagram(s), see printed CA Issue.

AB The estrogenic, antigonadotropic, ovulation inhibiting, and (or) blastocyte implantation inhibiting title compd. (I) was prepd. by the treatment of II (prepd. from 7.alpha.-methylestrone by known methods) with OsO4 in pyridine at room temp. in the dark followed by refluxing with NaHSO3 in EtOH. I was also prepd. by the redn. of III with LiAlH4 in refluxing THF.